# 2,3-Dichloropropyl isobutyrate

**Other names:** 1-Propanol, 2,3-dichloro, 2-methylpropanoate
**Inchi:** InChI=1S/C7H12Cl2O2/c1-5(2)7(10)11-4-6(9)3-8/h5-6H,3-4H2,1-2H3
**InchiKey:** QVKBGXGFHZCSQM-UHFFFAOYSA-N
**Formula:** C7H12Cl2O2
**SMILES:** CC(C)C(=O)OCC(Cl)CCl
**Mol. weight [g/mol]:** 199.07

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -254.60 | kJ/mol | Joback Method |
| hf | -474.65 | kJ/mol | Joback Method |
| hfus | 18.02 | kJ/mol | Joback Method |
| hvap | 48.33 | kJ/mol | Joback Method |
| log10ws | -1.79 | | Crippen Method |
| logp | 2.032 | | Crippen Method |
| mcvol | 141.410 | ml/mol | McGowan Method |
| pc | 2764.26 | kPa | Joback Method |
| rinpol | 1177.00 | | NIST Webbook |
| tb | 509.83 | K | Joback Method |
| tc | 706.13 | K | Joback Method |
| tf | 270.65 | K | Joback Method |
| vc | 0.537 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 291.25 | J/mol×K | 509.83 | Joback Method |
| cpg | 302.21 | J/mol×K | 542.55 | Joback Method |
| cpg | 312.68 | J/mol×K | 575.26 | Joback Method |
| cpg | 322.65 | J/mol×K | 607.98 | Joback Method |
| cpg | 332.13 | J/mol×K | 640.70 | Joback Method |
| cpg | 341.13 | J/mol×K | 673.41 | Joback Method |
| cpg | 349.65 | J/mol×K | 706.13 | Joback Method |
| dvisc | 0.0052697 | Pa×s | 270.65 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0022910 | Pa×s | 310.51 | Joback Method |
| dvisc | 0.0012039 | Pa×s | 350.38 | Joback Method |
| dvisc | 0.0007215 | Pa×s | 390.24 | Joback Method |
| dvisc | 0.0004754 | Pa×s | 430.10 | Joback Method |
| dvisc | 0.0003363 | Pa×s | 469.97 | Joback Method |
| dvisc | 0.0002511 | Pa×s | 509.83 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R34137&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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